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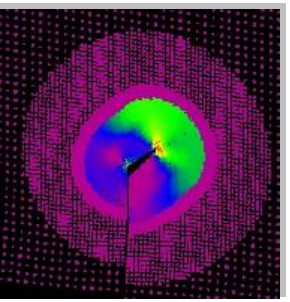
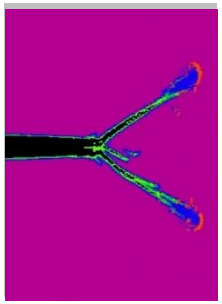
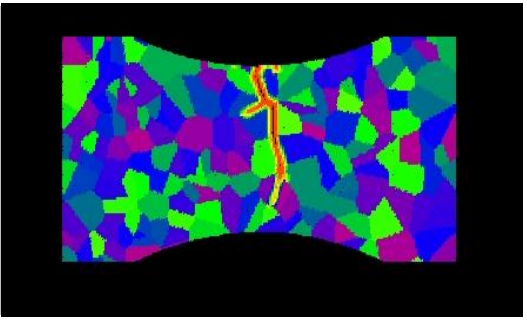

Defects and Interfaces in Peridynamics: A Multiscale Approach

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USACM Workshop on Meshfree Methods for Large-Scale Computational Science and Engineering

Tampa, FL

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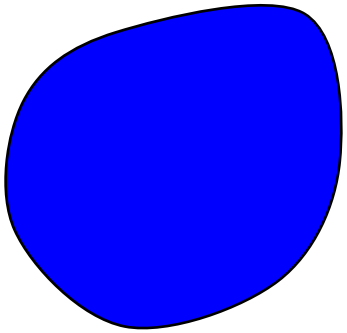
Outline

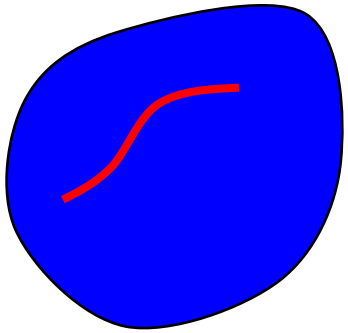
- Peridynamics background and examples
- Concurrent hierarchical multiscale method
- Calibrating a bond damage model using MD
- Coarse graining

Purpose of peridynamics*

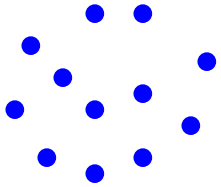
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



Continuous body



Continuous body with a defect

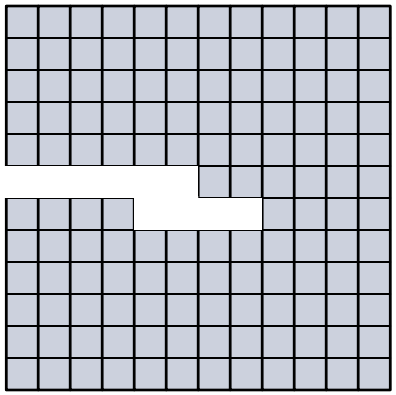


Discrete particles

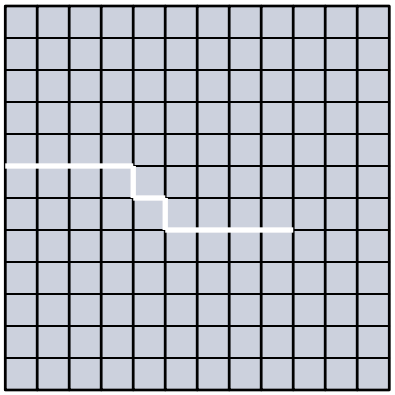
- Why do this?
  - Avoid coupling dissimilar mathematical systems (A to C).
  - Model complex fracture patterns.
  - Communicate across length scales.

* Peri (near) + dyn (force)

Some ways to treat cracks in an FE mesh



Element death



Cohesive interface elements

- Tend to get different results when you change the mesh.
- Methods do not reflect realistic crack-tip processes.
- Difficult to apply to complex crack trajectories.
- Methods destroy the accuracy and convergence properties of FEM.

Why do we have to do this sort of thing?
Because the equations that FEM approximate fail to apply.

Complex crack path in a composite

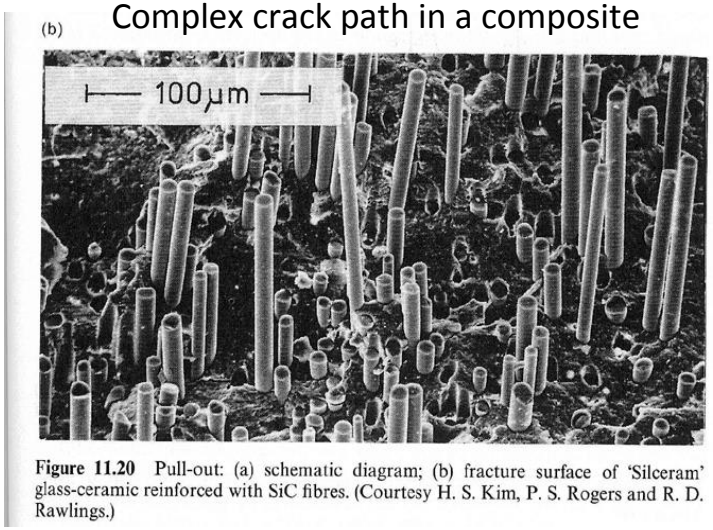
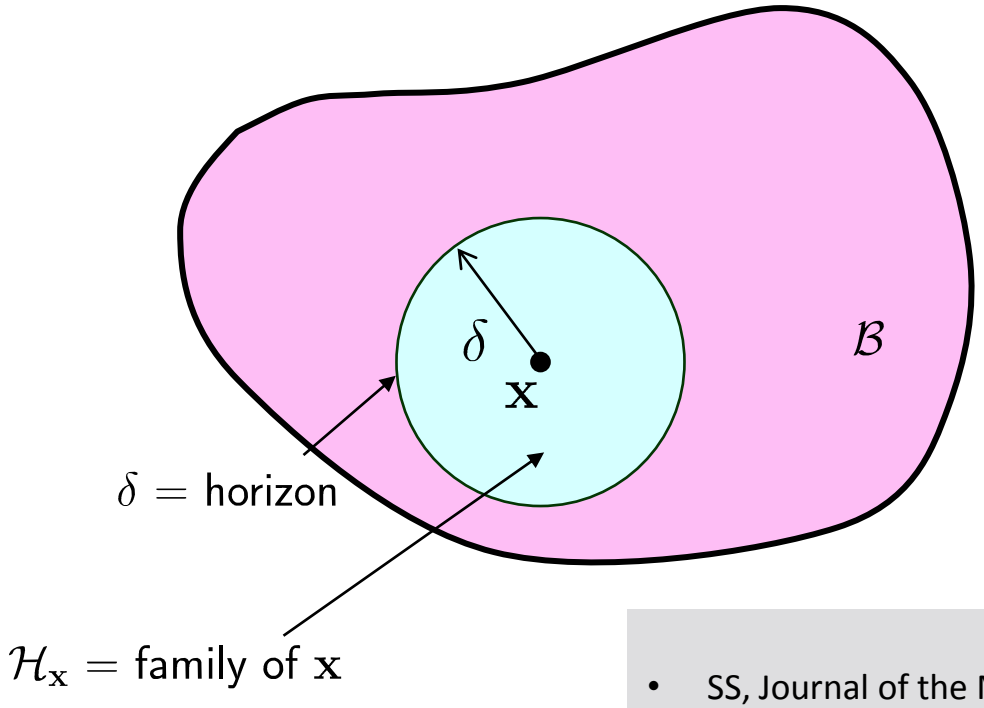


Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of 'Silceram' glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

Peridynamics basics: Horizon and family

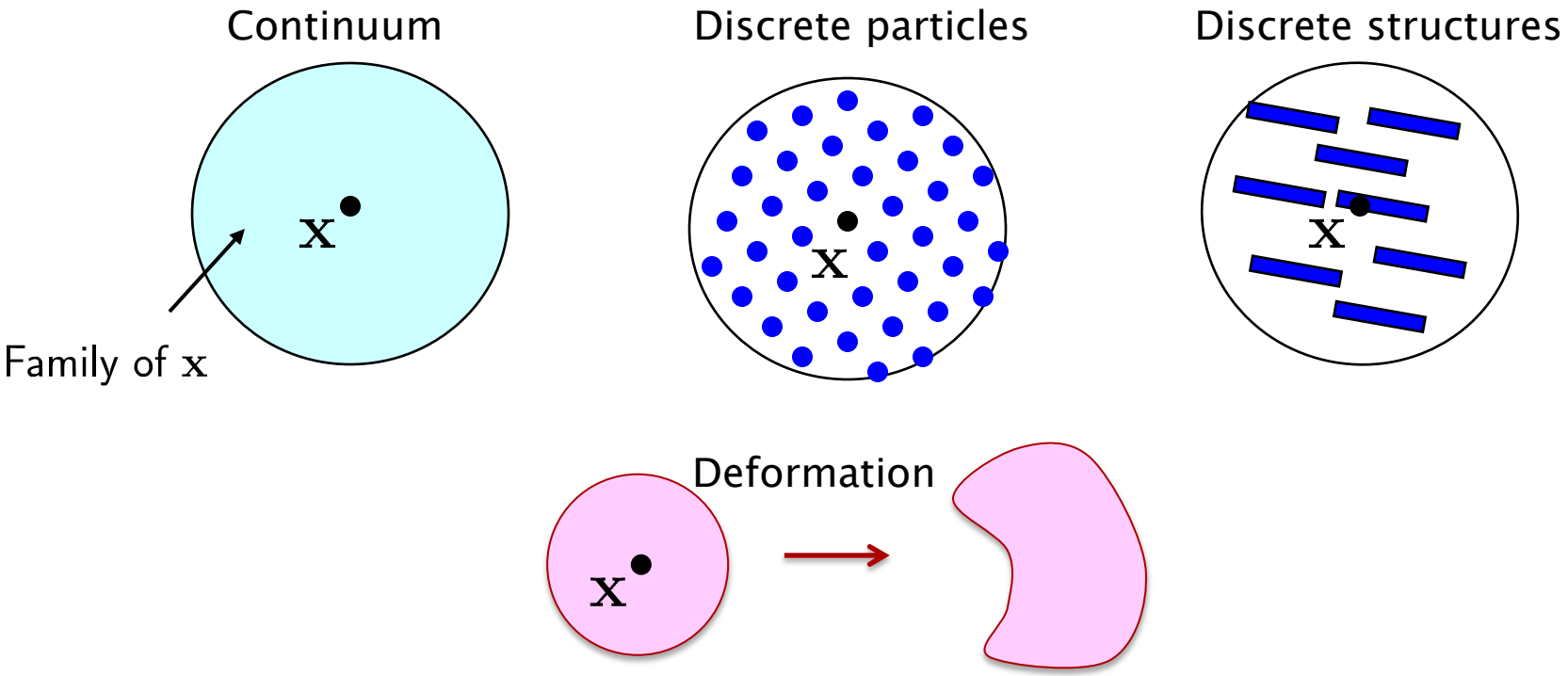
- Any point $\mathbf{x}$ interacts directly with other points within a distance δ called the "horizon."
- The material within a distance δ of $\mathbf{x}$ is called the "family" of $\mathbf{x}$, $\mathcal{H}_{\mathbf{x}}$.



General references

- SS, Journal of the Mechanics and Physics of Solids (2000)
- SS and R. Lehoucq, Advances in Applied Mechanics (2010)
- Madenci & Oterkus , *Peridynamic Theory & Its Applications* (2014)

Point of departure: Strain energy at a point



- Key assumption: the strain energy density at $\mathbf{x}$ is determined by the deformation of its family.

Potential energy minimization yields the peridynamic equilibrium equation

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- Potential energy:

$$\Phi = \int_{\mathcal{B}} (W - \mathbf{b} \cdot \mathbf{y}) \, dV_{\mathbf{x}}$$

  where W is the strain energy density, $\mathbf{y}$ is the deformation map, $\mathbf{b}$ is the applied external force density, and $\mathcal{B}$ is the body.

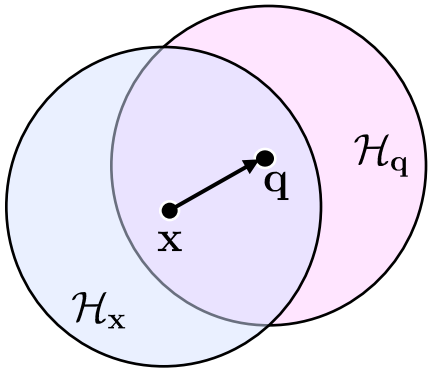
- Euler-Lagrange equation is the equilibrium equation:

$$\int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{q}, \mathbf{x}) \, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}) = 0$$

  for all $\mathbf{x}$. $\mathbf{f}$ is the *pairwise bond force density*.

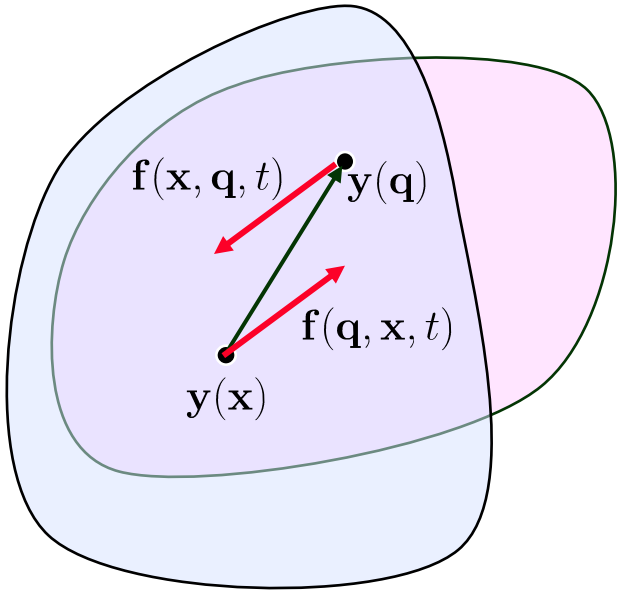
Peridynamics basics: Material model determines bond forces

- Each pairwise bond force vector $\mathbf{f}(\mathbf{q}, \mathbf{x}, t)$ is determined jointly by:
- the *collective* deformation of $\mathcal{H}_\mathbf{x}$, and
- the *collective* deformation of $\mathcal{H}_\mathbf{q}$.
- Bond forces are antisymmetric: $\mathbf{f}(\mathbf{x}, \mathbf{q}, t) = -\mathbf{f}(\mathbf{q}, \mathbf{x}, t)$.



Undeformed families

Deformation $\mathbf{y}(\cdot, t)$



Deformed families and bond forces

Peridynamics basics:
The nature of internal forces

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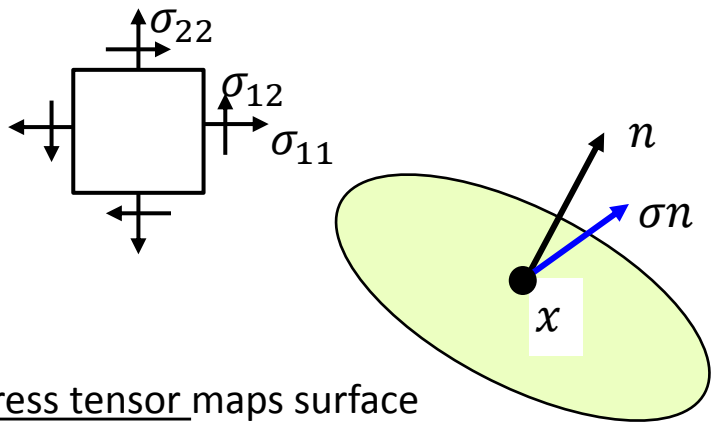
Standard theory

Stress tensor field
(assumes continuity of forces)



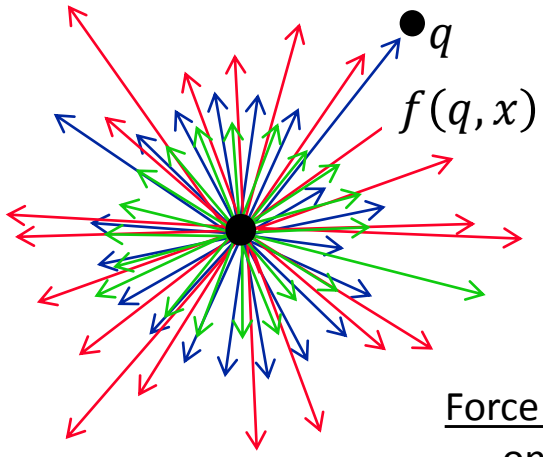
Stress tensor maps surface normal vectors onto surface forces

$$\rho\ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t)$$

Differentiation of surface forces

Peridynamics

Bond forces between neighboring points
(allowing discontinuity)



Force state maps bonds onto bond forces

$$\rho\ddot{u}(x,t) = \int_{H_x} f(q,x)dV_q + b(x,t)$$

Summation over bond forces

Peridynamic vs. local equations

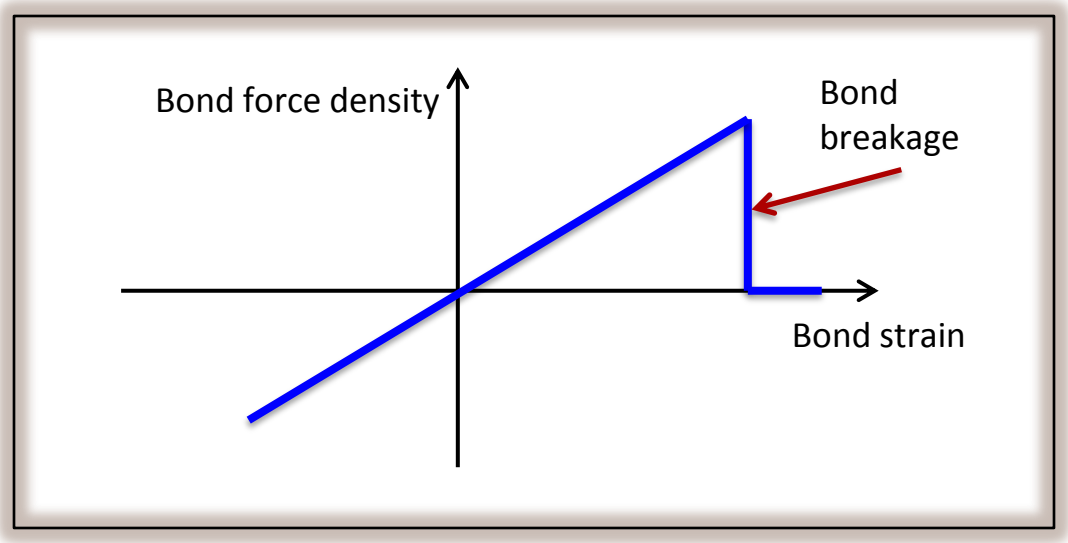
- The structures of the theories are similar, but peridynamics uses nonlocal operators.

Relation	*Peridynamic theory*	*Standard theory*
Kinematics	$\underline{\mathbf{Y}}\langle \mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q})-\mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \dfrac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \displaystyle\int_{\mathcal{H}} \Big(\mathbf{t}(\mathbf{q},\mathbf{x}) - \mathbf{t}(\mathbf{x},\mathbf{q})\Big)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\mathbf{t}(\mathbf{q},\mathbf{x}) = \underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle, \qquad \underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$
Angular momentum balance	$\displaystyle\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle \mathbf{q}-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle\, dV_{\mathbf{q}} = \mathbf{0}$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{\mathbf{Y}}}$ (Fréchet derivative)	$\boldsymbol{\sigma} = W_{\mathbf{F}}$ (tensor gradient)
First law	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} + q + r$	$\dot{\varepsilon} = \boldsymbol{\sigma}\cdot\dot{\mathbf{F}} + q + r$

$$\underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} := \int_{\mathcal{H}} \underline{\mathbf{T}}\langle \boldsymbol{\xi}\rangle \cdot \underline{\dot{\mathbf{Y}}}\langle \boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}}$$

Bond based material models

- If each bond response is independent of the others, the resulting material model is called bond-based.
- The material model is then simply a graph of bond force density vs. bond strain.
- Damage can be modeled through bond breakage.
- Bond response is calibrated to:
  - Bulk elastic properties.
  - Critical energy release rate.



Linearized theory

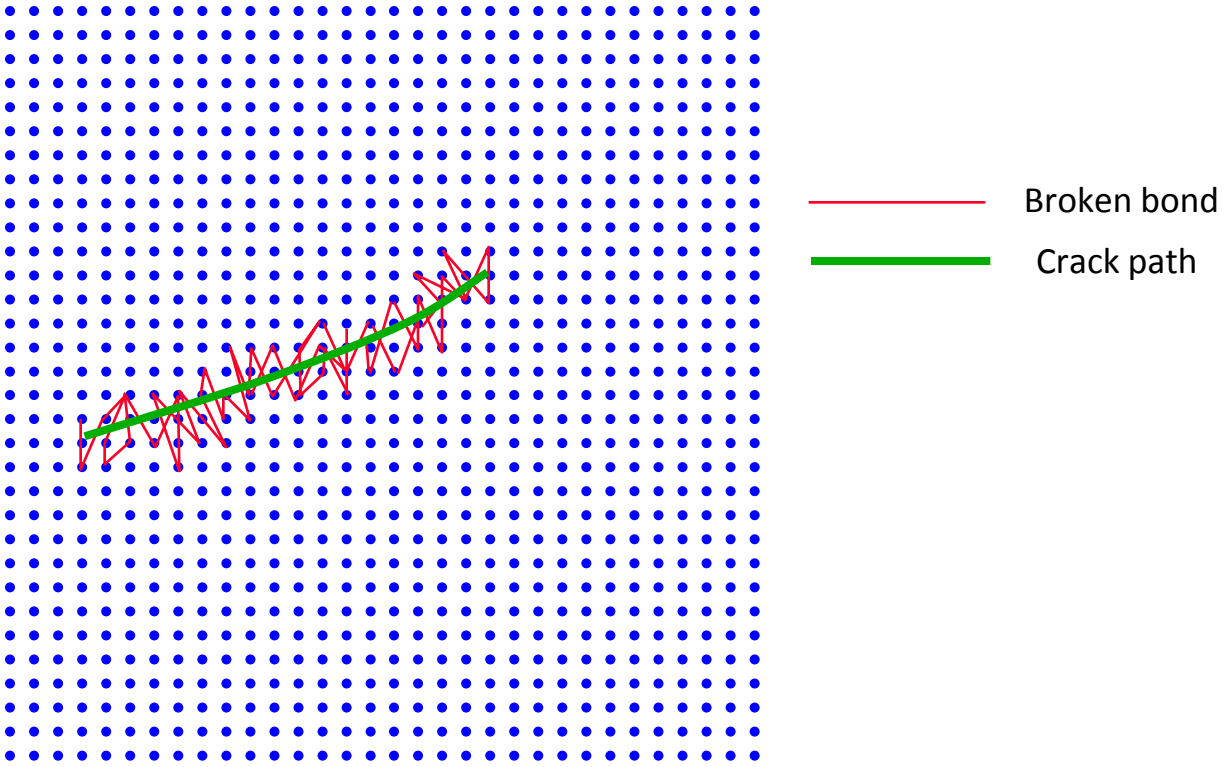
- For small displacements (possibly superposed on a large deformation):

$$\rho\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{C}(\mathbf{x},\mathbf{q})(\mathbf{u}(\mathbf{q},t) - \mathbf{u}(\mathbf{x},t))\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x},t)$$

  where $\mathbf{C}$ is the tensor-valued *micromodulus* field.

- Equation is formally the same as in Kunin's nonlocal theory.
- Can still have bond breakage.
- Most of the following discussion uses the linearized theory.
- Will see how to get $\mathbf{C}$ by multiscale methods.

Autonomous crack growth



- When a bond breaks, its load is shifted to its neighbors, leading to progressive failure.

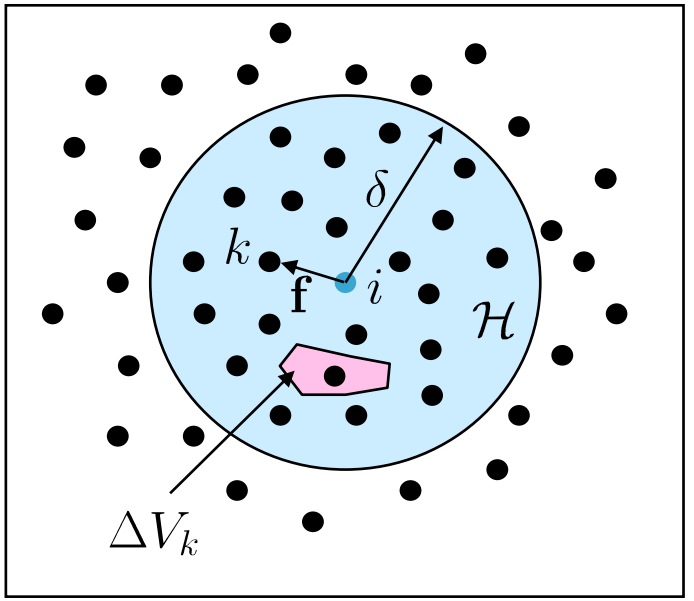
EMU numerical method

- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t) \quad \longrightarrow \quad \rho\ddot{\mathbf{y}}_i^n = \sum_{k\in\mathcal{H}} \mathbf{f}(\mathbf{x}_k,\mathbf{x}_i,t)\, \Delta V_k + \mathbf{b}_i^n$$

- Linearized model:

$$\rho\ddot{\mathbf{u}}_i = \sum_{k\in\mathcal{H}_i} \mathbf{C}_{ik}(\mathbf{u}_k - \mathbf{u}_i)\Delta V_k + \mathbf{b}_i$$



Peridynamics fun facts

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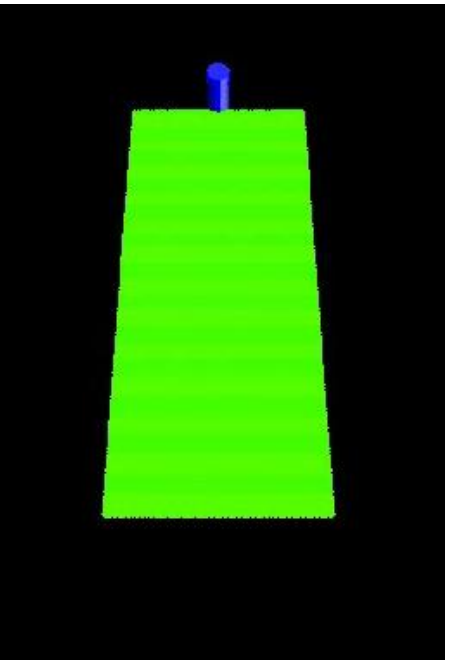
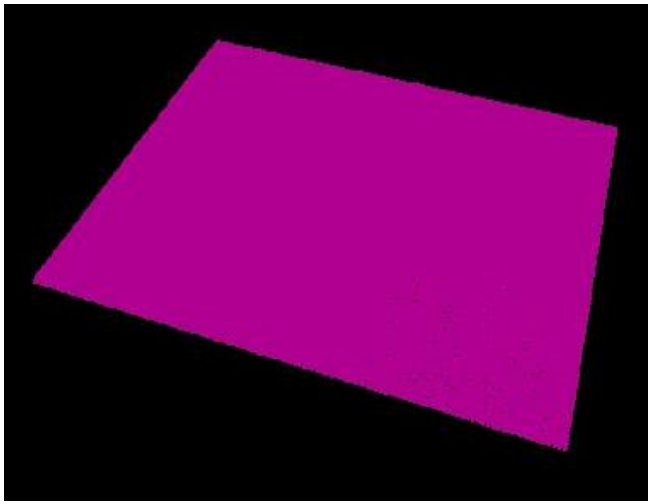
- Molecular dynamics is a special case of peridynamics
  - Any multibody potential can be made into a peridynamic material model (Seleson & Parks, 2014).
- Classical (local) PDEs are a limiting case of peridynamics as $\delta \to 0$ (SS & Lehoucq, 2008).
- Any material model from the classical theory can be included.
  - e.g., Strain-hardening viscoplastic (Foster & Chen, 2010.)
  - Classical material models with the Emu discretization are similar to
    - RKPM (Bessa, Foster, Belytschko, & Liu, 2014).
    - SPH (Ganzenmüller, Hiermaier, & May, 2014).
- Waves are dispersive
  - Material properties can be deduced from dispersion curves (Weckner & SS, 2011).
- It's possible to model crack nucleation and growth without damage (!).
  - Use nonconvex bond energy (Lipton, 2014).

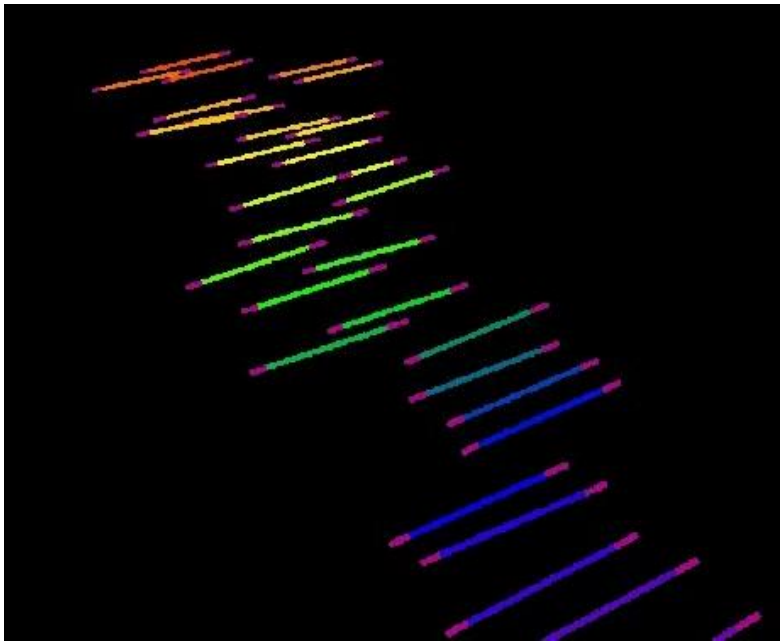
Examples: Membranes and thin structures (videos)



Oscillatory crack path



Crack interaction in a sheet



Self-assembly

Dynamic crack branching

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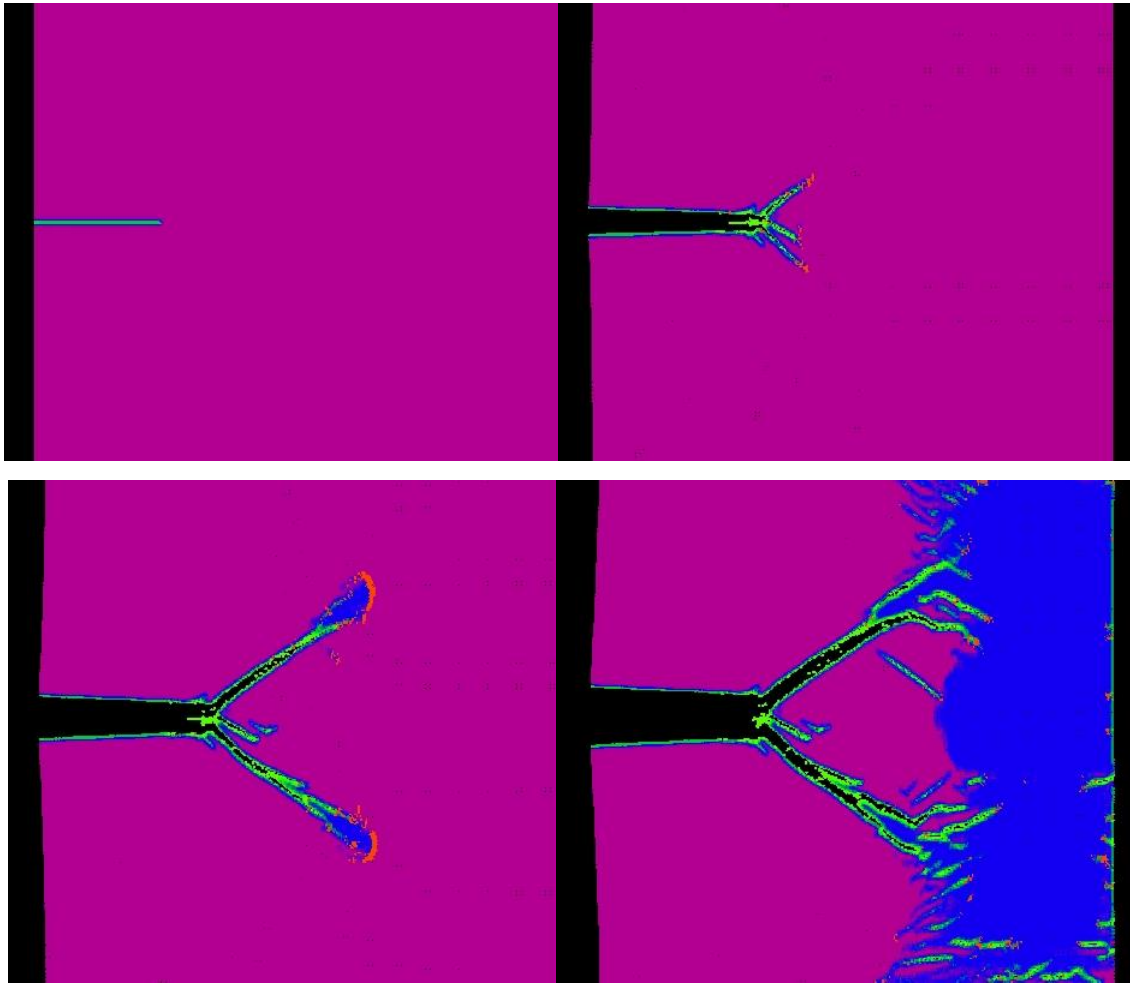
- Similar to previous example but with higher strain rate applied at the boundaries.
- Red indicates bonds currently undergoing damage.
    - These appear ahead of the visible discontinuities.
- Blue/green indicate damage (broken bonds).
- More and more energy is being built up ahead of the crack – it can't keep up.
    - Leads to fragmentation.



More on dynamic fracture: see Ha & Bobaru (2010, 2011)

Dynamic crack branching (video)

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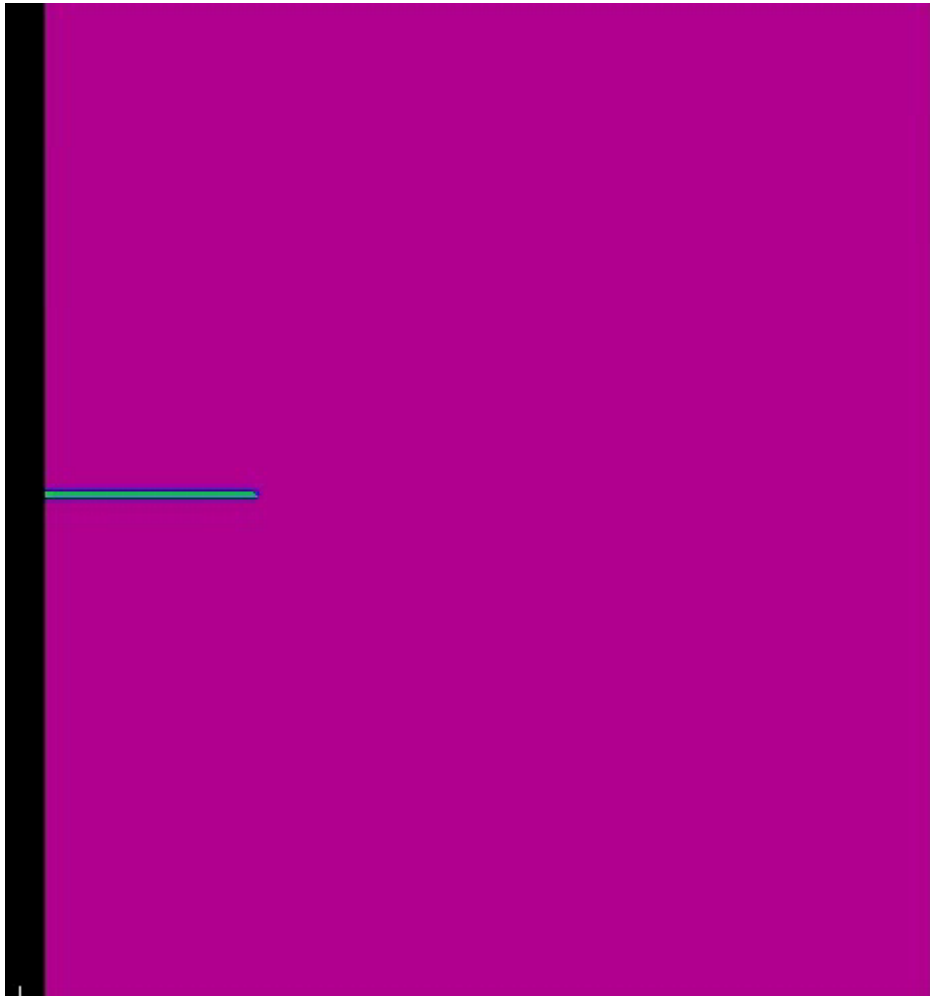

More on dynamic fracture: see Ha & Bobaru (2010, 2011)

Some peridynamic multiscale methods and results

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- Derivation of peridynamic equations from statistical mechanics (Lehoucq & Sears, 2011).
- Higher order gradients to connect MD to peridynamic (Seleson, Parks, Gunzburger, & Lehoucq, 2005).
- Adaptive mesh refinement (Bobaru & Hu, 2011).
- Coarse-graining (SS, 2011).
- Two-scale evolution equation for composites (Alali & Lipton, 2012).
- PFHMM method for atomistic-to-continuum coupling (Rahman, Foster, & Haque, 2014).

Concurrent multiscale method for defects

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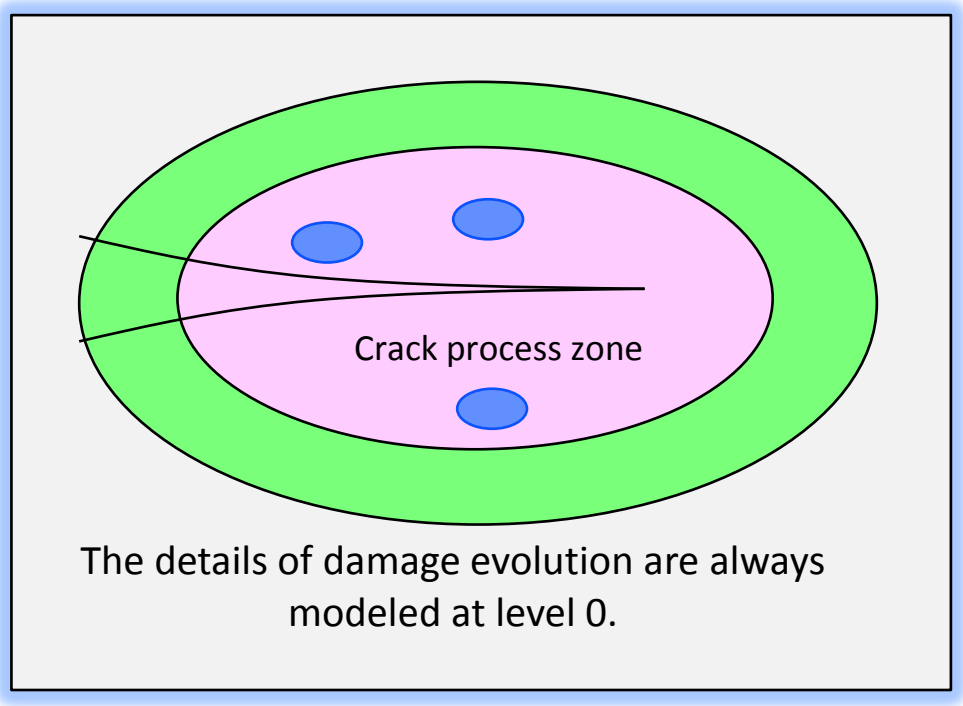
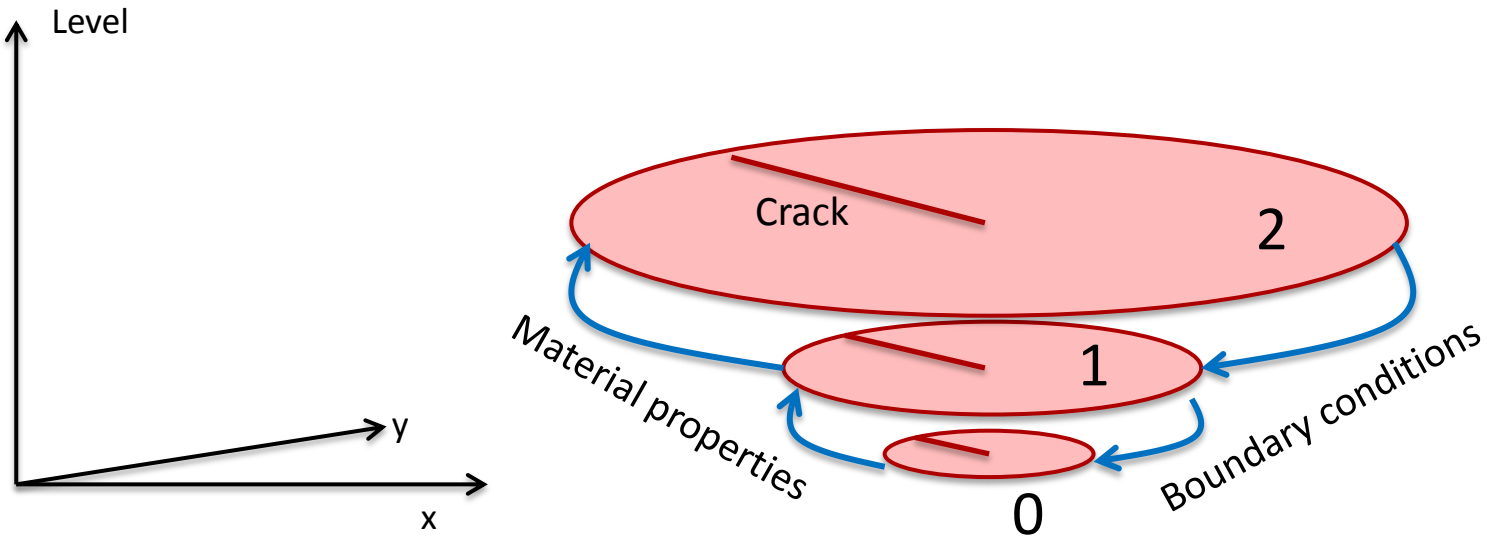
- Apply the best practical physics at the smallest length scale (near a crack tip).
- Scale up hierarchically to larger length scales.
- Each level is related to the one below it by the same equations.
  - Any number of levels can be used.
- Adaptively follow the crack tip.



Concurrent solution strategy

- The equation of motion is applied only within each level.
- Higher levels provide boundary conditions on lower levels.
- Lower levels provide coarsened material properties (including damage) to higher levels.



Schematic of communication between levels in a 2D body

Concurrent multiscale example: shear loading of a crack

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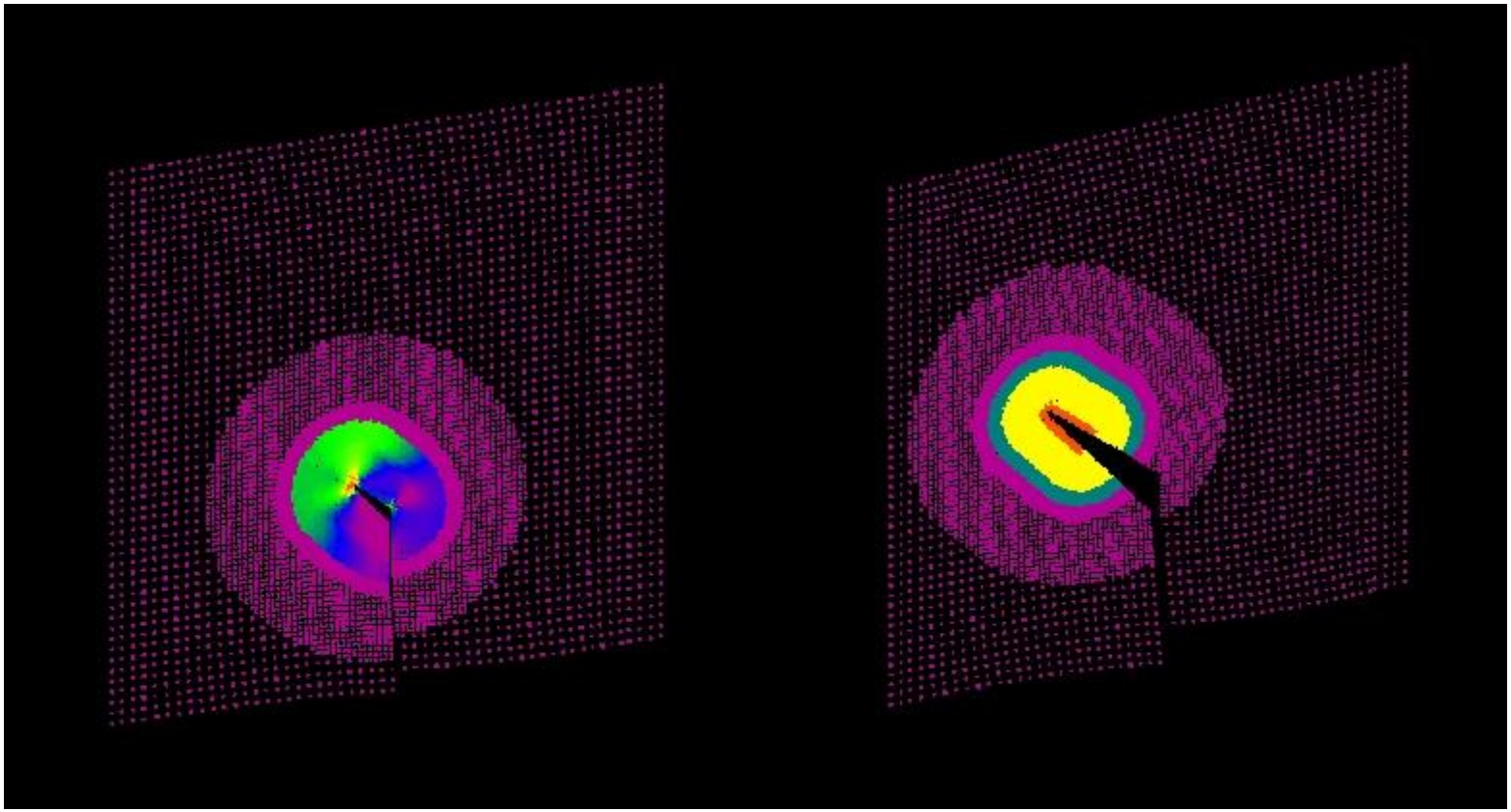

Bond strain

Damage process zone

Multiscale crack growth in a heterogeneous medium (video)

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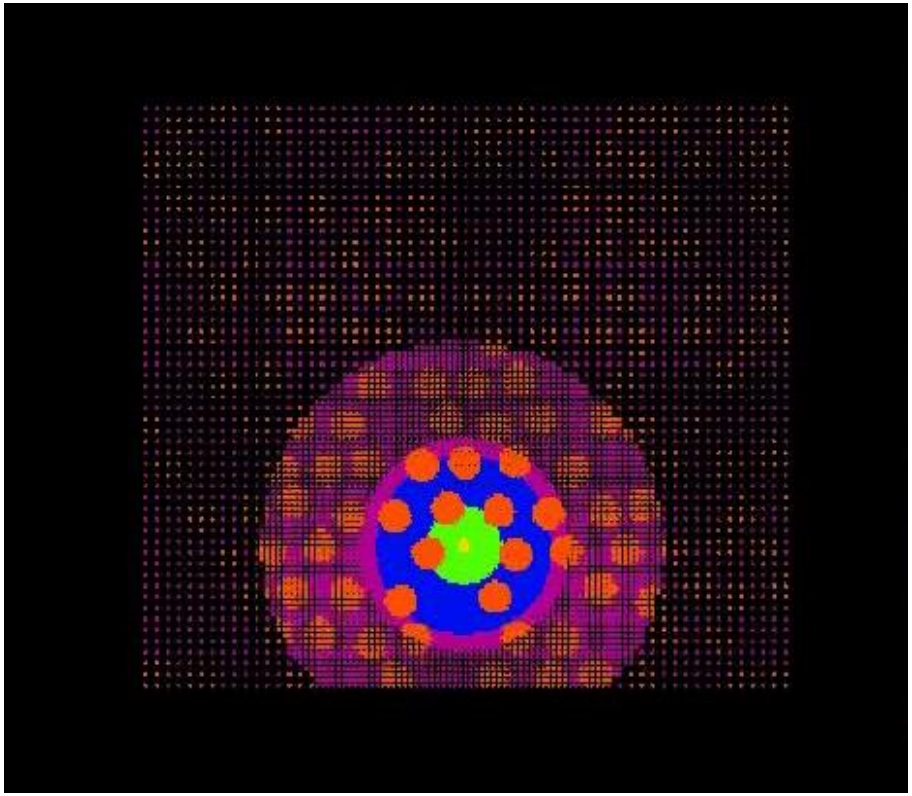

Branching in a heterogeneous medium

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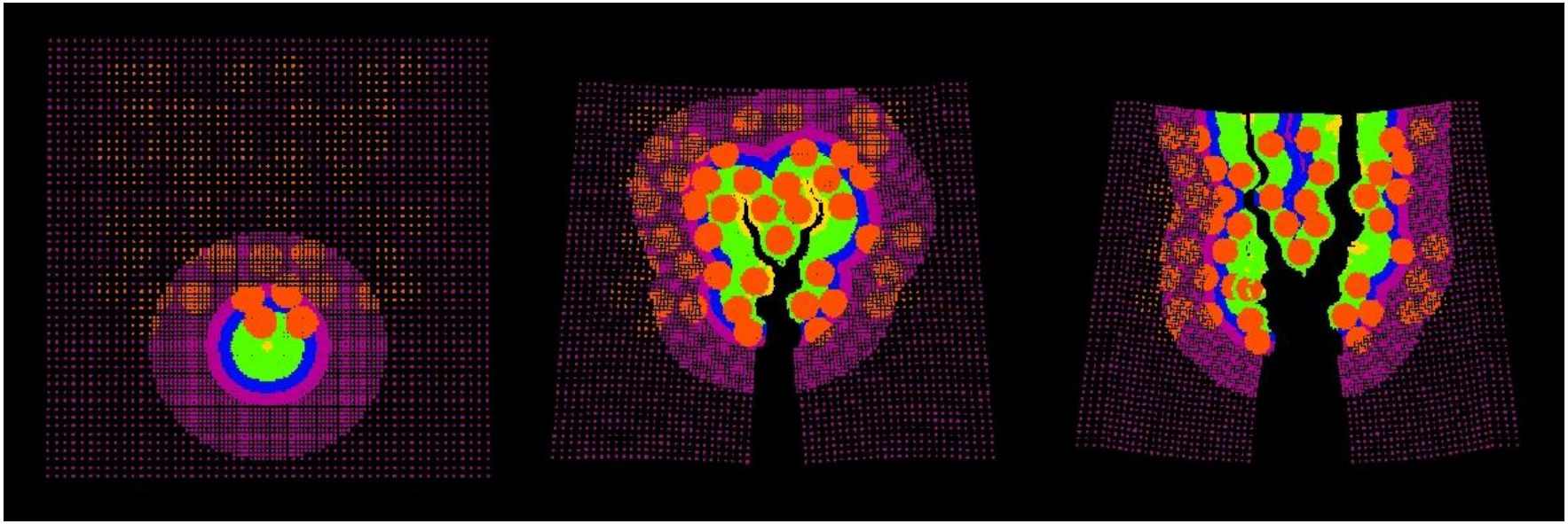
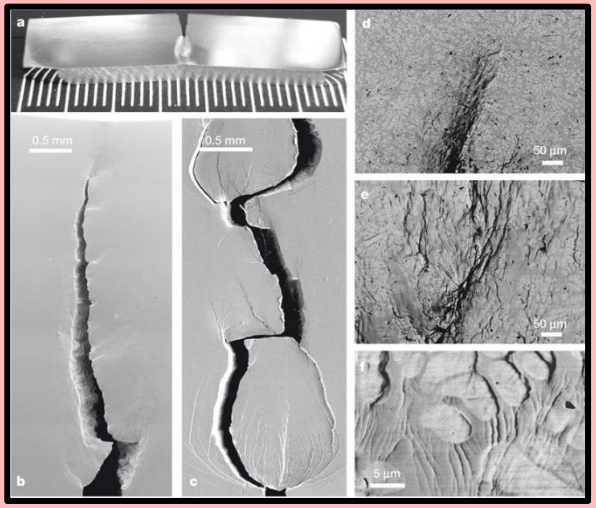
- Crack grows between randomly placed hard inclusions.



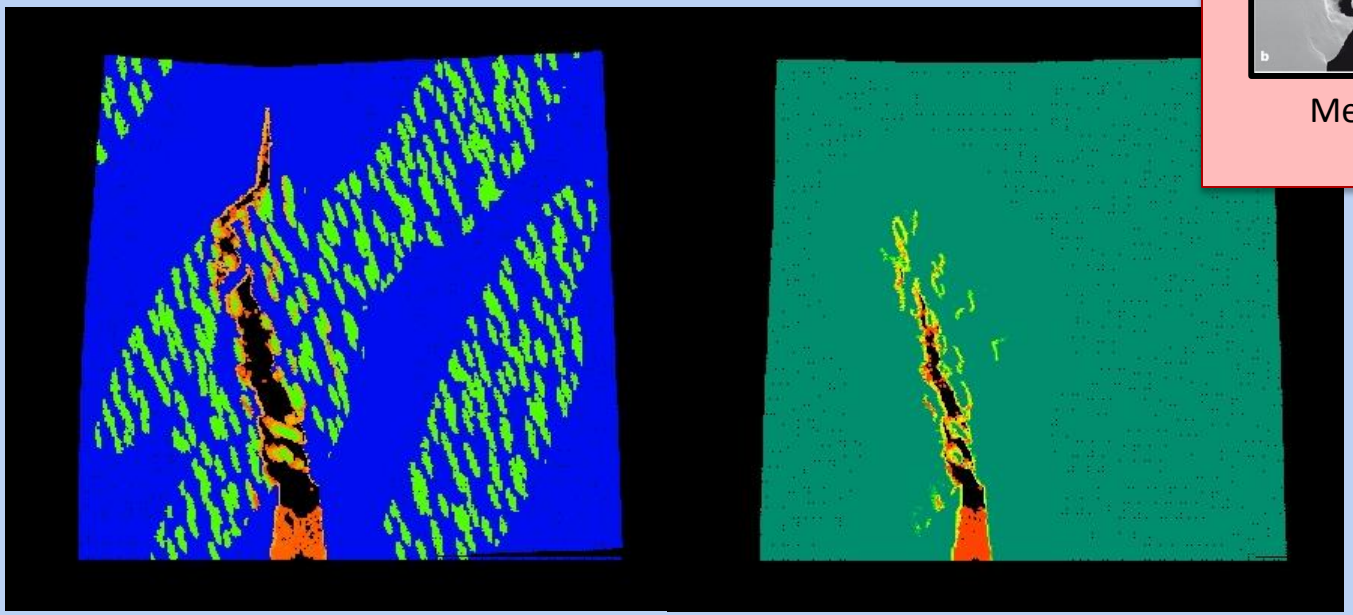
Multiscale modeling reveals the structure of brittle cracks

- Material design requires understanding of how morphology at multiple length scales affects strength.
- This is a key to material reliability.



Metallic glass fracture (Hofmann et al, Nature 2008)

Multiscale model of crack growth through a brittle material with distributed defects



Upscaling of material properties

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- Suppose we have an accurate model in level 0.
  - How can we obtain material properties in level 1?
  - This is sometimes called “coarse-graining”.
  - Will next describe a method for doing this based on constrained optimization.

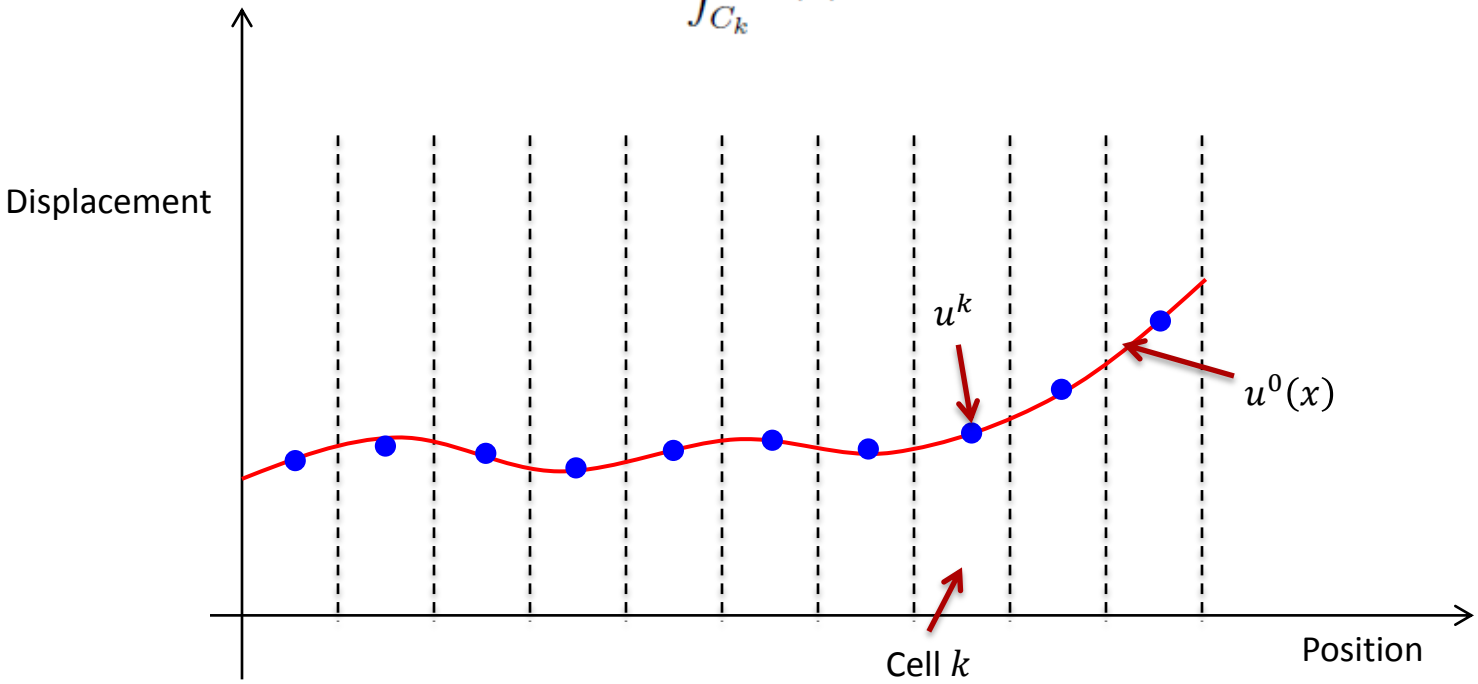
Level 1 DOFs

- Divide the region into K "cells" C_k.
- The mean level 0 displacement within each cell is the level 1 DOF:

$$u_k^1 = \int_{C_k} \varphi(x) u^0(x)\, dx$$

where

$$\int_{C_k} \varphi(x) = 1.$$



Level 1 DOF as a constraint

- Pretend all the u_k^1 values are given.
- In effect, this places a constraint on the u^0 function.
- Constrained potential energy functional:

$$\Phi = \int_{\mathcal{B}} (W^0(x) - u^0(x)b(x))\, dx - \sum_{k=1}^{K} \lambda_k \left(\int_{C_k} \varphi(x) u^0(x)\, dx - u_k^1 \right)$$

where $\lambda_1, \lambda_2, \ldots, \lambda_K$ are Lagrange multipliers.

Force balance on cell k

- Resulting constrained equilibrium equation:

$$L^0(x) + b(x) + \lambda_k \varphi(x) = 0$$

where k is whichever cell contains x and L^0 is the level 0 internal force operator:

$$L^0(x) = \int_{\mathcal{H}_\mathbf{x}} \left(\underline{T}[x]\langle q - x \rangle - \underline{T}[q]\langle x - q \rangle \right) dq.$$

- Observe that the constraint acts like a body force distributed over cell k.
- Integrate the equilibrium equation over cell k, recall $\int \varphi = 1$, set $b \equiv 0$:

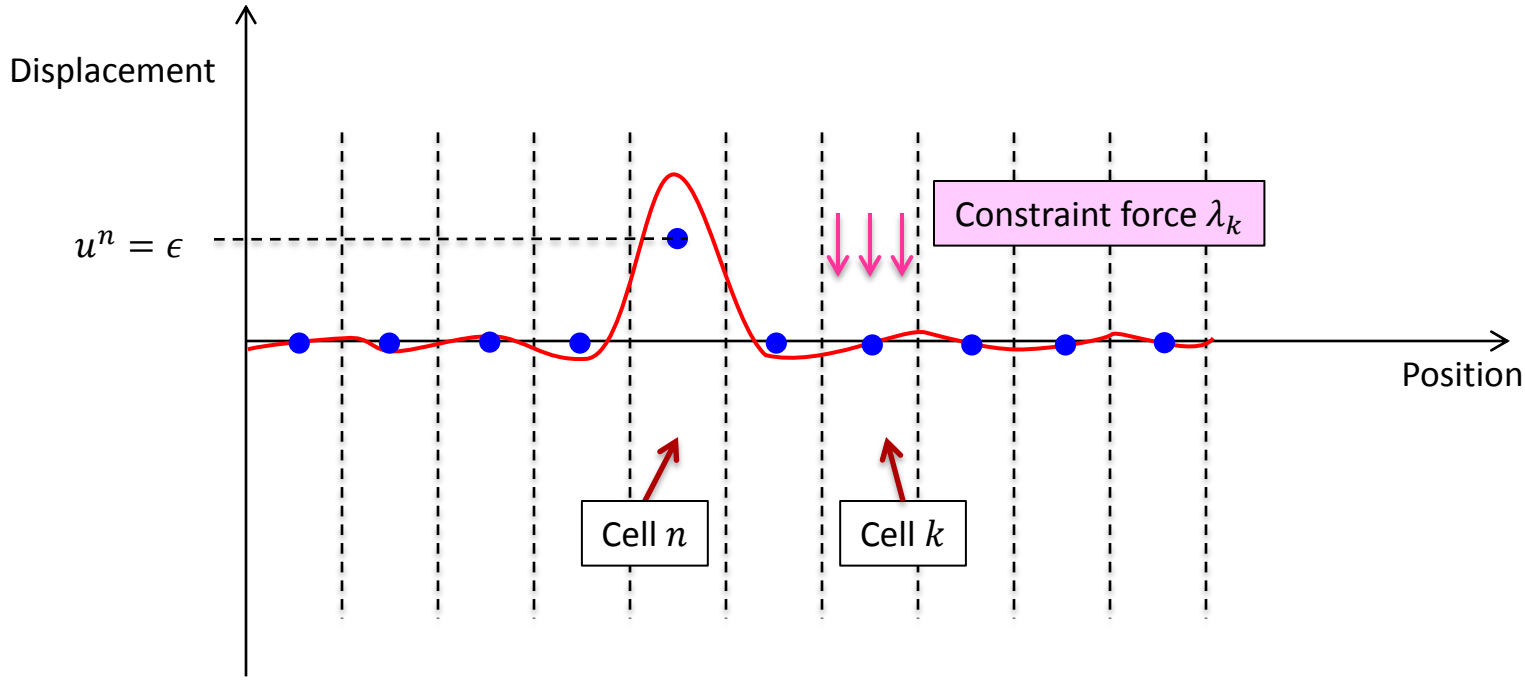
$$\int_{C_k} L^0(x)\, dx + \lambda_k = 0.$$

Interaction forces from other cells + constraint force = 0

Level 1 micromodulus

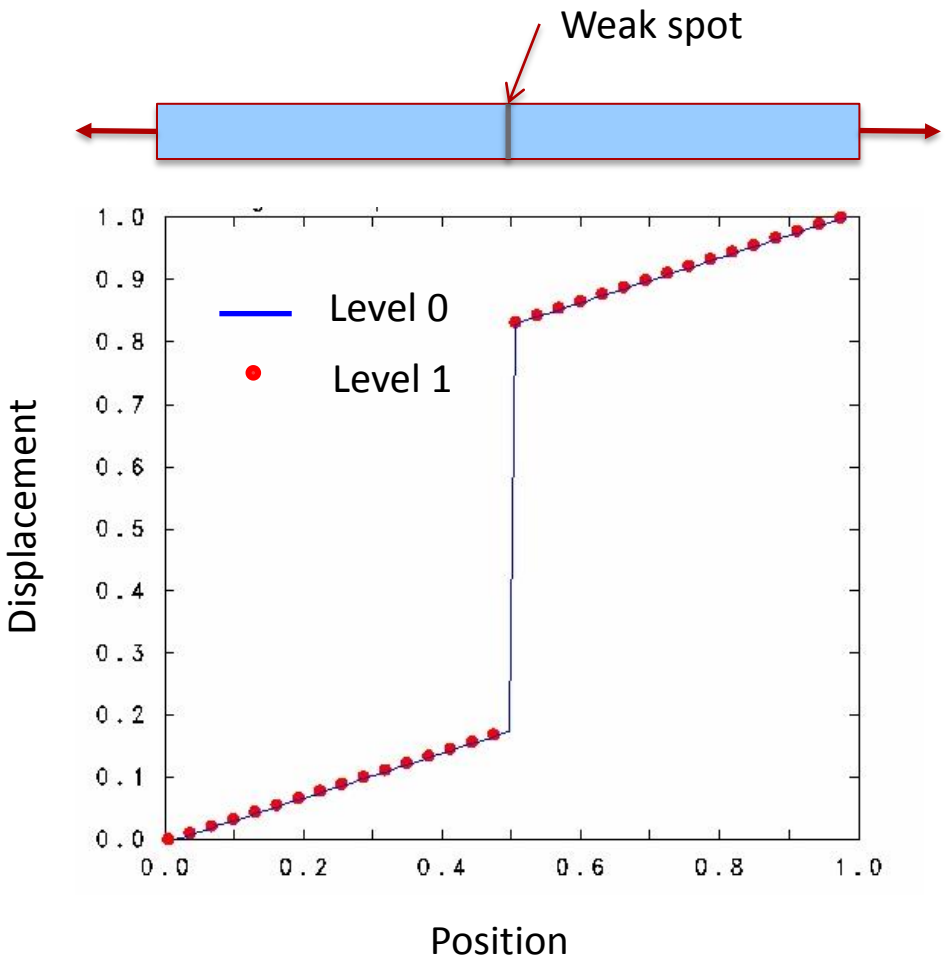
- Set all $u_k^1 = 0$ except for cell n: $u_n^1 = \epsilon \ll 1$.
- Solve the constrained equilibrium equation for $u^0(x)$ and the $\lambda_1, \lambda_2, \ldots, \lambda_K$.
- The upscaled micromodulus is

$$c_{kn}^1 = \lambda_k / \epsilon.$$



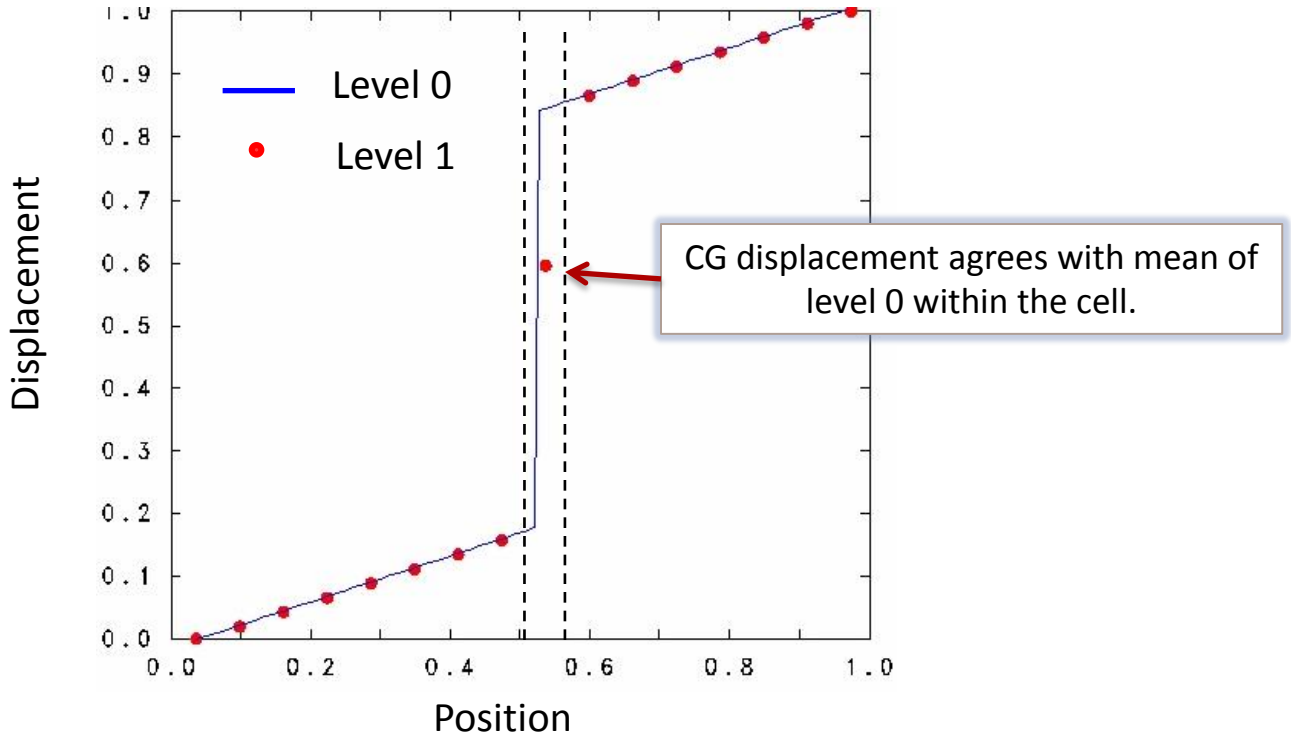
Example: Rod with a defect

- Upscaling method preserves the effect of a defect embedded within a cell.



Coarser level 1

- If the defect is not exactly at a cell boundary, the method still produces the mean of the level 0 displacements within each cell.

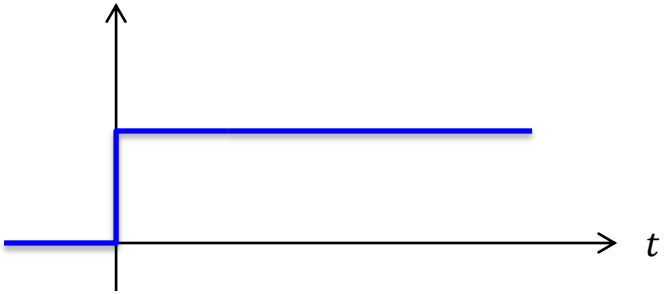


Time-dependent response

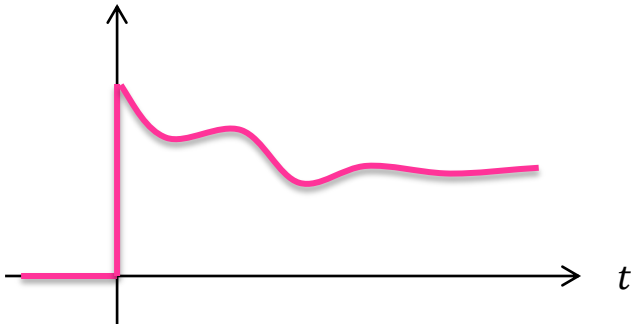
- Time-dependent bond force model for level 1:

$$f(x_n, x_k) = \int_0^t \lambda_k(t-\tau)(\dot{u}(x_k,\tau) - \dot{u}(x_n,\tau))\, d\tau$$

$\epsilon(t)$= cell n displacement

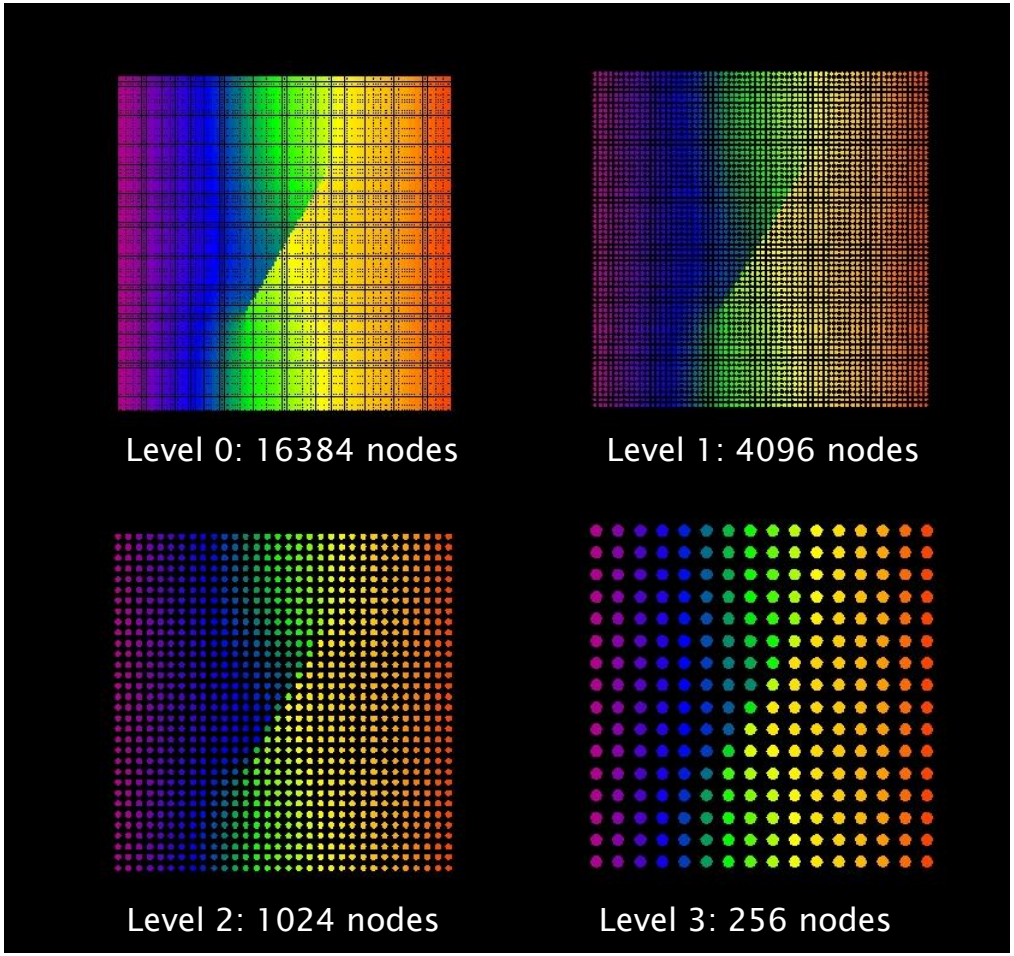


$\lambda_k(t)$= cell k constraint force



Coarse graining verification: crack in a plate

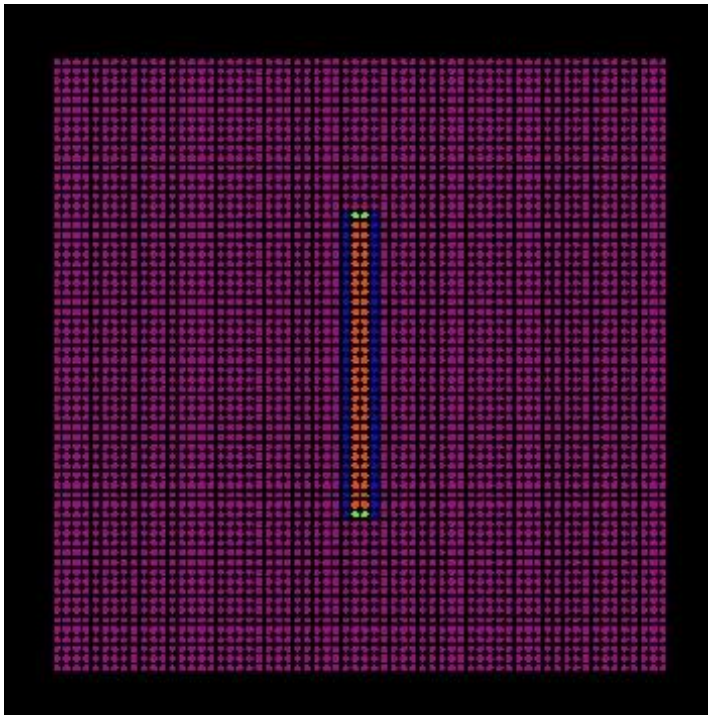
- Example: Solve the same problem in four different levels using the successively upscaled material properties – results are the same.



Defining damage from coarse-grained material properties

Sandia National Laboratories

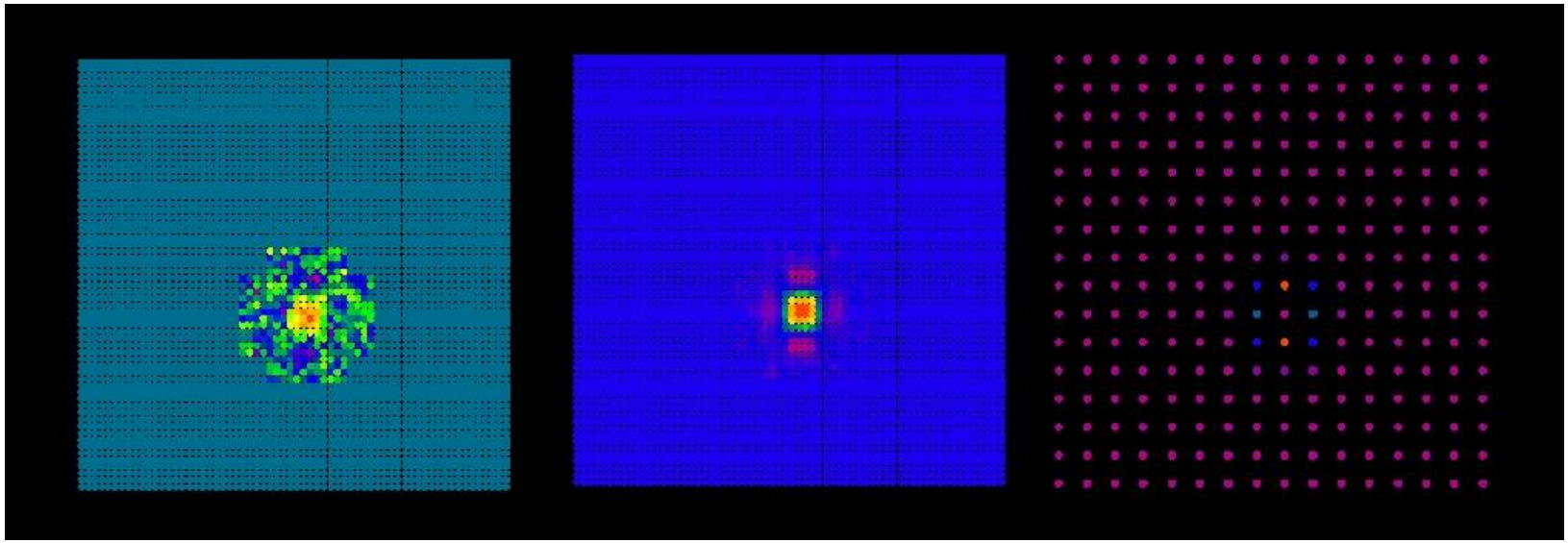
- Define bonds to be damaged if their coarse-grained micromodulus is less than a tolerance.
- This allows damage to be determined without deforming the MD grid.



Level 1 damage contours deduced from coarse-grained properties

Coarse graining MD directly into peridynamics

- The level 0 physics can be anything: PD, standard continuum, MD, MC(?), DFT(?)



Level 0: MD showing thermal oscillations

MD time-averaged displacements

Level 1: Coarse grained micromodulus

Summary

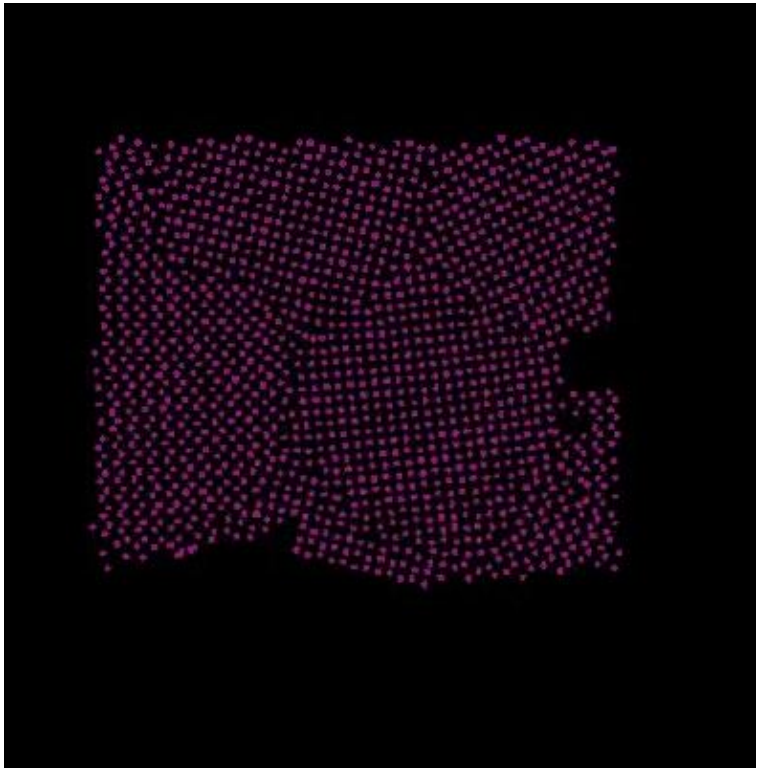
- Concurrent multiscale:
  - Adaptively follow crack tips.
  - Apply the best practical physics in level 0.
  - MD time step is impractical. Instead…
- Calibrate a peridynamic damage model from an MD simulation.
  - Derives continuum damage parameters (“parameter passing”).
- Coarse-graining:
  - Derives incremental elastic properties at higher levels.
  - Does not rely on a representative volume element (RVE).

- Methods are “scalable:” can be applied any number of times to obtain any desired increase in length scale.

Level 0: calibrating a peridynamic model using molecular dynamics

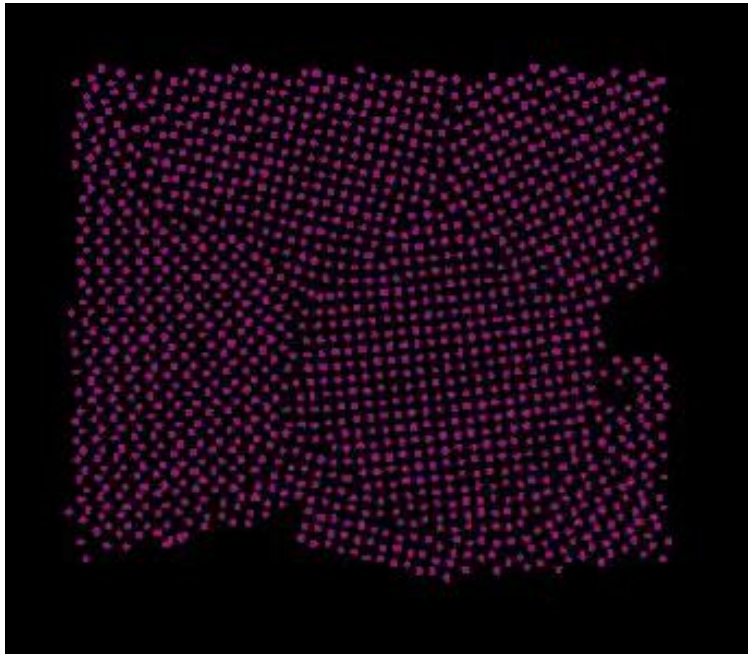
- The concurrent multiscale method, in spite of subcycling the lower levels, is still not efficient enough to use MD in level 0 for growing cracks.
- Instead: Use MD to calibrate a continuum model.

- Video show smoothed atomic positions in a LAMMPS model of Al polycrystal (courtesy David Newsome, CFD Research Corp.)
- Yellow-red: bond strains > 1.0.



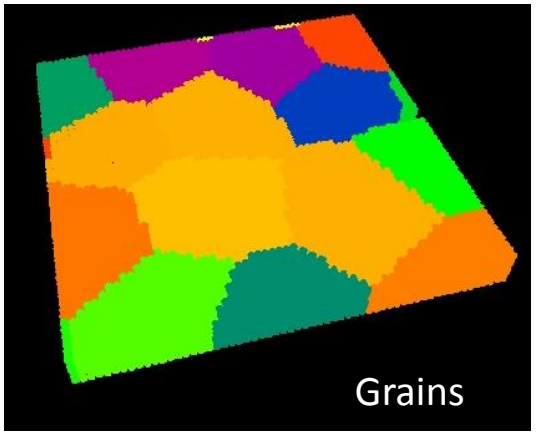
Peridynamic mesoscale simulations using properties determined from MD

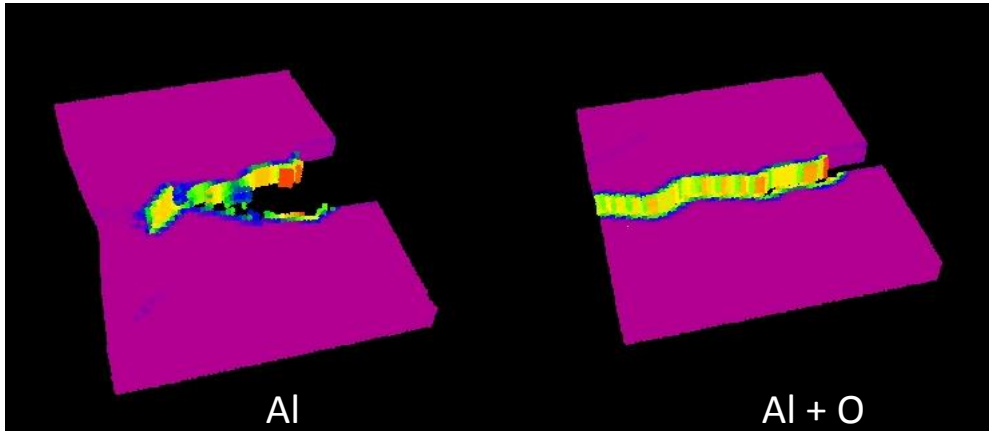
- Continuum model of a polycrystal shows the effect of embrittlement due to oxide.



Time-averaged atomic positions (LAMMPS).
Colors = peridynamic bond strain.

Calibrated peridynamic bond interactions





Colors indicate damage (broken bonds)